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                 Web Page for STN Seminar Schedule - N. America
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NEWS 3
         AUG 06
                 FSTA enhanced with new thesaurus edition
NEWS
         AUG 13
                 CA/CAplus enhanced with additional kind codes for granted
                 patents
         AUG 20
NEWS
                 CA/CAplus enhanced with CAS indexing in pre-1907 records
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         AUG 27
                 Full-text patent databases enhanced with predefined
                 patent family display formats from INPADOCDB
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         AUG 27
                 USPATOLD now available on STN
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         SEP 13
NEWS 12 SEP 17
                 CA/CAplus enhanced with printed CA page images from
                 1967-1998
NEWS 13
         SEP 17
                 CAplus coverage extended to include traditional medicine
                 patents
NEWS 14 SEP 24
                 EMBASE, EMBAL, and LEMBASE reloaded with enhancements
NEWS 15 OCT 02
                 CA/CAplus enhanced with pre-1907 records from Chemisches
                 Zentralblatt
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NEWS 22 DEC 17 USPATOLD added to additional database clusters
NEWS 23 DEC 17
                 IMSDRUGCONF removed from database clusters and STN
NEWS 24 DEC 17
                 DGENE now includes more than 10 million sequences
NEWS 25
         DEC 17
                 TOXCENTER enhanced with 2008 MeSH vocabulary in
                 MEDLINE segment
NEWS 26
         DEC 17
                 MEDLINE and LMEDLINE updated with 2008 MeSH vocabulary
         DEC 17
NEWS 27
                 CA/CAplus enhanced with new custom IPC display formats
NEWS 28
         DEC 17
                 STN Viewer enhanced with full-text patent content
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              19 SEPTEMBER 2007: CURRENT WINDOWS VERSION IS V8.2,
              CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP),
              AND CURRENT DISCOVER FILE IS DATED 19 SEPTEMBER 2007.
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2-11 3-13 5-10 6-7 7-9
1-2 1-6 2-3 3-4 4-5 5-6
2-11 3-13 5-10 6-7 7-9
1-2 1-6 2-3 3-4 4-5 5-6
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1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 7:CLASS 9:Atom 10:CLASS 11:CLASS

chain nodes : 7 9 10 11 13 ring nodes : 1 2 3 4 5 6 chain bonds :

ring bonds :

G1:0,S,N G2:C,O,S

Match level :

Generic attributes :

L1 STRUCTURE UPLOADED

STR

: Unsaturated

13:CLASS

Saturation

=> d 11

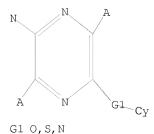
L1

L1 HAS NO ANSWERS

9:

exact/norm bonds :

normalized bonds :



Structure attributes must be viewed using STN Express query preparation.

=> s 11
SAMPLE SEARCH INITIATED 07:17:26 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 1270 TO ITERATE

100.0% PROCESSED 1270 ITERATIONS 2 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 23263 TO 27537
PROJECTED ANSWERS: 2 TO 124

L2 2 SEA SSS SAM L1

=> s l1 sss full

FULL SEARCH INITIATED 07:17:31 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 25778 TO ITERATE

100.0% PROCESSED 25778 ITERATIONS 50 ANSWERS

SEARCH TIME: 00.00.01

L3 50 SEA SSS FUL L1

=> file caplus

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 ENTRY
 SESSION

 FULL ESTIMATED COST
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 172.31

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=> s 13

7 L3 L4

=> d 1-7 ibib abs hitstr

L4 ANSWER 1 OF 7 CAPLUS COPYRIGHT 2007 ACS on STN

2007:351030 CAPLUS ACCESSION NUMBER:

DOCUMENT NUMBER: 146:380011

TITLE: Preparation of N-pyrazinyl phenylsulfonamides as

chemokine receptor modulators for treatment of asthma

INVENTOR(S): Kindon, Nicholas; Mete, Antonio; Teobald, Barry

Astrazeneca AB, Swed. PATENT ASSIGNEE(S): PCT Int. Appl., 79pp. SOURCE:

CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PAT	ENT	NO.			KIN:	D	DATE			APPL	ICAT	ION	NO.		D	ATE	
WO	2007	0351	 54		A1	_		0329	,	WO 2	006-	SE10	60		21	00609	918
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		GE,	GH,	GM,	HN,	HR,	ΗU,	ID,	IL,	IN,	IS,	JP,	ΚE,	KG,	KΜ,	KN,	KP,
		KR,	KΖ,	LA,	LC,	LK,	LR,	LS,	LT,	LU,	LV,	LY,	MA,	MD,	MG,	MK,	MN,
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		IS,	ΙT,	LT,	LU,	LV,	MC,	NL,	PL,	PT,	RO,	SE,	SI,	SK,	TR,	BF,	ВJ,
		CF,	CG,	CI,	CM,	GΑ,	GN,	GQ,	GW,	ML,	MR,	ΝE,	SN,	TD,	TG,	BW,	GH,
		GM,	ΚE,	LS,	MW,	ΜZ,	NA,	SD,	SL,	SZ,	TZ,	UG,	ZM,	ZW,	AM,	AZ,	BY,
		KG,	KΖ,	MD,	RU,	ΤJ,	TM										
PRIORITY	APP	LN.	INFO	.:						SE 2	005-	2068			A 20	00509	919
OTHER SOURCE(S):				MAR:	MARPAT 146:380011												

GI

AB The title N-pyrazinyl phenylsulfonamides I [wherein R1 = H, Me, F, or C1; one of R2 and R3 = H or F; the other of R2 and R3 = (un)substituted CH2NH2 or CH2CH2NH2] or pharmaceutically acceptable salts thereof were prepared as chemokine receptor modulators for treatment of asthma (no data). For example, II was prepared in a multi-step synthesis. II showed 96.4% binding activity towards human plasma protein.

IT 931092-38-5P 931092-41-0P 931092-48-7P 931092-61-4P 931092-62-5P 931092-67-0P 931092-68-1P 931092-72-7P 931092-73-8P 931092-78-3P 931092-78-3P 931092-81-8P 931092-82-9P 931092-86-3P 931092-87-4P 931092-88-5P 931092-92-1P 931093-00-4P 931093-07-1P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(drug candidate; preparation of N-pyrazinyl phenylsulfonamides as chemokine receptor modulators for treatment of asthma)

RN 931092-38-5 CAPLUS

CN Benzenesulfonamide, N-[5-[4-[(1R)-1-aminoethyl]phenoxy]-3-methoxy-6-methyl-2-pyrazinyl]-2,3-dichloro-, hydrochloride (1:?) (CA INDEX NAME)

Absolute stereochemistry.

●x HCl

RN 931092-41-0 CAPLUS

CN Benzenesulfonamide, N-[5-[3-[(1S)-1-aminoethyl]phenoxy]-3-methoxy-6-methyl-2-pyrazinyl]-2,3-dichloro- (CA INDEX NAME)

Absolute stereochemistry.

RN 931092-48-7 CAPLUS

CN Benzenesulfonamide, N-[5-[4-[(1S)-1-aminoethyl]phenoxy]-3-methoxy-6-methyl-2-pyrazinyl]-2,3-dichloro-, hydrochloride (1:?) (CA INDEX NAME)

Absolute stereochemistry.

●x HCl

RN 931092-61-4 CAPLUS

CN Benzenesulfonamide, N-[5-[4-[(1S)-1-amino-2-hydroxyethyl]phenoxy]-3-methoxy-6-methyl-2-pyrazinyl]-2,3-dichloro- (CA INDEX NAME)

Absolute stereochemistry.

RN 931092-62-5 CAPLUS

CN Benzenesulfonamide, N-[5-[4-[(1S)-1-amino-2-hydroxyethyl]phenoxy]-3-methoxy-6-methyl-2-pyrazinyl]-2,3-dichloro-, 2,2,2-trifluoroacetate (1:?) (CA INDEX NAME)

CM 1

CRN 931092-61-4 CMF C20 H20 C12 N4 O5 S

Absolute stereochemistry.

CM 2

CRN 76-05-1 CMF C2 H F3 O2

$$\begin{array}{c} F \\ | \\ C - CO_2H \\ | \\ F \end{array}$$

RN 931092-67-0 CAPLUS

CN Benzenesulfonamide, 2,3-dichloro-N-[6-chloro-3-methoxy-5-[4-[(1R)-1-(methylamino)ethyl]phenoxy]-2-pyrazinyl]- (CA INDEX NAME)

Absolute stereochemistry.

RN 931092-68-1 CAPLUS

CN Benzenesulfonamide, 2,3-dichloro-N-[6-chloro-3-methoxy-5-[4-[(1R)-1-(methylamino)ethyl]phenoxy]-2-pyrazinyl]-, 2,2,2-trifluoroacetate (1:?) (CA INDEX NAME)

CM 1

CRN 931092-67-0

CMF C20 H19 C13 N4 O4 S

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 931092-72-7 CAPLUS

CN Benzenesulfonamide, 2,3-dichloro-N-[3-methoxy-6-methyl-5-[4-[(1R)-1-(methylamino)ethyl]phenoxy]-2-pyrazinyl]- (CA INDEX NAME)

Absolute stereochemistry.

RN 931092-73-8 CAPLUS

CN Benzenesulfonamide, 2,3-dichloro-N-[3-methoxy-6-methyl-5-[4-[(1R)-1-(methylamino)ethyl]phenoxy]-2-pyrazinyl]-, 2,2,2-trifluoroacetate (1:?) (CA INDEX NAME)

CM 1

CRN 931092-72-7

CMF C21 H22 C12 N4 O4 S

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 931092-78-3 CAPLUS

CN Benzenesulfonamide, N-[5-[4-[(1S)-1-amino-2-hydroxyethy1]phenoxy]-6-chloro-3-methoxy-2-pyraziny1]-2,3-dichloro- (CA INDEX NAME)

Absolute stereochemistry.

RN 931092-79-4 CAPLUS

CN Benzenesulfonamide, N-[5-[4-[(1S)-1-amino-2-hydroxyethyl]phenoxy]-6-chloro-3-methoxy-2-pyrazinyl]-2,3-dichloro-, 2,2,2-trifluoroacetate (1:?) (CA INDEX NAME)

CM 1

CRN 931092-78-3

CMF C19 H17 C13 N4 O5 S

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 931092-80-7 CAPLUS

CN Benzenesulfonamide, N-[5-[4-[(1R)-1-aminoethyl]phenoxy]-6-fluoro-3-methoxy-2-pyrazinyl]-2,3-dichloro-, hydrochloride (1:?) (CA INDEX NAME)

Absolute stereochemistry.

●x HCl

RN 931092-81-8 CAPLUS

CN Benzenesulfonamide, N-[5-[4-[(1S)-1-amino-2-hydroxyethyl]phenoxy]-6-fluoro-3-methoxy-2-pyrazinyl]-2,3-dichloro- (CA INDEX NAME)

RN 931092-82-9 CAPLUS

CN Benzenesulfonamide, N-[5-[4-[(1\$)-1-amino-2-hydroxyethyl]phenoxy]-6-fluoro-3-methoxy-2-pyrazinyl]-2,3-dichloro-, 2,2,2-trifluoroacetate (1:?) (CA INDEX NAME)

CM 1

CRN 931092-81-8

CMF C19 H17 C12 F N4 O5 S

Absolute stereochemistry.

CM 2

CRN 76-05-1 CMF C2 H F3 O2

$${\tiny \begin{array}{c}F\\F-C-co_2H\\|\\F\end{array}}$$

RN 931092-86-3 CAPLUS

CN Benzenesulfonamide, N-[5-[4-[(1R)-1-amino-2-hydroxyethyl]phenoxy]-3-methoxy-6-methyl-2-pyrazinyl]-2,3-dichloro- (CA INDEX NAME)

RN 931092-87-4 CAPLUS

CN Benzenesulfonamide, N-[5-[4-[(1R)-1-amino-2-hydroxyethyl]phenoxy]-3-methoxy-6-methyl-2-pyrazinyl]-2,3-dichloro-, 2,2,2-trifluoroacetate (1:?) (CA INDEX NAME)

CM 1

CRN 931092-86-3

CMF C20 H20 C12 N4 O5 S

Absolute stereochemistry.

CM 2

CRN 76-05-1 CMF C2 H F3 O2

$$\begin{array}{c} F \\ | \\ F - C - CO_2H \\ | \\ F \end{array}$$

RN 931092-88-5 CAPLUS

CN Benzenesulfonamide, N-[5-[4-[(1S)-1-aminoethy1]phenoxy]-6-fluoro-3-methoxy-2-pyraziny1]-2,3-dichloro- (CA INDEX NAME)

RN 931092-92-1 CAPLUS

CN Benzenesulfonamide, N-[5-[4-[(1R)-1-aminoethyl]phenoxy]-3-methoxy-6-methyl-2-pyrazinyl]-2,3-dichloro- (CA INDEX NAME)

Absolute stereochemistry.

RN 931093-00-4 CAPLUS

CN Benzenesulfonamide, N-[5-[4-[(1S)-1-aminoethyl]phenoxy]-3-methoxy-6-methyl-2-pyrazinyl]-2,3-dichloro- (CA INDEX NAME)

Absolute stereochemistry.

RN 931093-07-1 CAPLUS

CN Benzenesulfonamide, N-[5-[4-[(1R)-1-aminoethyl]phenoxy]-6-fluoro-3-methoxy-2-pyrazinyl]-2,3-dichloro- (CA INDEX NAME)

IT 931093-14-0P 931093-24-2P 931093-25-3P

931093-28-6P 931093-29-7P 931093-36-6P

931093-41-3P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(intermediate; preparation of N-pyrazinyl phenylsulfonamides as chemokine receptor modulators for treatment of asthma)

RN 931093-14-0 CAPLUS

CN Carbamic acid, N-[(1S)-1-[3-[[5-[[(2,3-dichlorophenyl)sulfonyl]][[2-(trimethylsilyl)ethoxy]methyl]amino]-6-methoxy-3-methyl-2-pyrazinyl]oxy]phenyl]ethyl]-, 1,1-dimethylethyl ester (CA INDEX NAME)

Absolute stereochemistry.

RN 931093-24-2 CAPLUS

CN Carbamic acid, N-[(1R)-1-[4-[[3-chloro-5-[[(2,3-dichlorophenyl)sulfonyl][[2-(trimethylsilyl)ethoxy]methyl]amino]-6-methoxy-2-pyrazinyl]oxy]phenyl]ethyl]-, 1,1-dimethylethyl ester (CA INDEX NAME)

RN 931093-25-3 CAPLUS

CN Carbamic acid, N-[(1R)-1-[4-[[3-chloro-5-[[(2,3-dichlorophenyl)sulfonyl][[2-(trimethylsilyl)ethoxy]methyl]amino]-6-methoxy-2-pyrazinyl]oxy]phenyl]ethyl]-N-methyl-, 1,1-dimethylethyl ester (CA INDEX NAME)

Absolute stereochemistry.

RN 931093-28-6 CAPLUS

CN Carbamic acid, N-[(1R)-1-[4-[[5-[[(2,3-dichlorophenyl)sulfonyl]][[2-(trimethylsilyl)ethoxy]methyl]amino]-6-methoxy-3-methyl-2-pyrazinyl]oxy]phenyl]ethyl]-, 1,1-dimethylethyl ester (CA INDEX NAME)

Absolute stereochemistry.

RN 931093-29-7 CAPLUS

CN Carbamic acid, N-[(1R)-1-[4-[[5-[[(2,3-dichlorophenyl)sulfonyl]][[2-(trimethylsilyl)ethoxy]methyl]amino]-6-methoxy-3-methyl-2-pyrazinyl]oxy]phenyl]ethyl]-N-methyl-, 1,1-dimethylethyl ester (CA INDEX

NAME)

Absolute stereochemistry.

RN 931093-36-6 CAPLUS

CN Carbamic acid, N-[(1R)-1-[4-[[5-[[(2,3-dichlorophenyl)sulfonyl]][[2-(trimethylsilyl)ethoxy]methyl]amino]-3-fluoro-6-methoxy-2-pyrazinyl]oxy]phenyl]ethyl]-, 1,1-dimethylethyl ester (CA INDEX NAME)

Absolute stereochemistry.

RN 931093-41-3 CAPLUS

CN Carbamic acid, N-[(1S)-1-[4-[[5-[[(2,3-dichlorophenyl)sulfonyl]][[2-(trimethylsilyl)ethoxy]methyl]amino]-3-fluoro-6-methoxy-2-pyrazinyl]oxy]phenyl]ethyl]-, 1,1-dimethylethyl ester (CA INDEX NAME)

Absolute stereochemistry.

REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 2 OF 7 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2004:252506 CAPLUS

DOCUMENT NUMBER: 140:287400

TITLE: Preparation of substituted 1,4-pyrazine derivatives as

CRF inhibitors

INVENTOR(S): Corbett, Jeffrey W.; Fu, Jian-min; Ennis, Michael D.;

Frank, Kristine E.; Hoffman, Robert L.; Verhoest,

Patrick R.

PATENT ASSIGNEE(S): Pharmacia & Upjohn Company, USA

SOURCE: PCT Int. Appl., 42 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

P	ATENT	NO.			KIN	D	DATE								D.	ATE	
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OTHER SOURCE(S): MARPAT 140:287400

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AB Title compds. I [X = (un)substituted amino, alkoxy, alkyl, acyl, etc.; V = 0, amino, SO0-2; R1-2 = (un)substituted amino, alkoxy, halo, alkyl, etc.; Ar = (hetero)aryl] are prepared For instance, 3-chloro-2,5-diethylpyrazine is coupled to (1R,2S)-1-amino-2-indanol (PhMe, NaOBu-t, Pd2dba3, 100°, 2 h). The resulting adduct is iodinated (DMSO, I2) and coupled to 2-hydroxy-4-methylpyridine (DMF, CuI, Cs2CO3, 80°) to give II. I are inhibitors of corticotropin releasing factor and are useful in treating anxiety disorders, depression and stress related disorders.

II

IT 675198-65-9P, (1R,2S)-1-[[3,6-Diethyl-5-[(4-methylpyridin-2-yl)oxy]pyrazin-2-yl]amino]-2,3-dihydro-1H-inden-2-ol 675198-72-8P, (1R,2S)-1-[[3,6-Diethyl-5-[(4-ethylpyridin-2-yl)oxy]pyrazin-2-yl]amino]indan-2-ol 675198-76-2P, (1R,2S)-1-[[3,6-Diethyl-5-[(5-methylpyridin-2-yl)oxy]pyrazin-2-yl]amino]indan-2-ol RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

(preparation of substituted 1,4-pyrazine derivs. as CRF inhibitors) 675198-65-9 CAPLUS

CN 1H-Inden-2-ol, 1-[[3,6-diethyl-5-[(4-methyl-2-pyridinyl)oxy]pyrazinyl]amino]-2,3-dihydro-, (1R,2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN

RN 675198-72-8 CAPLUS

CN 1H-Inden-2-ol, 1-[[3,6-diethyl-5-[(4-ethyl-2-pyridinyl)oxy]pyrazinyl]amino]-2,3-dihydro-, (1R,2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 675198-76-2 CAPLUS

CN 1H-Inden-2-ol, 1-[[3,6-diethyl-5-[(5-methyl-2-pyridinyl)oxy]pyrazinyl]amino]-2,3-dihydro-, (1R,2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN

IT 675198-67-1P 675198-68-2P 675198-69-3P
675198-70-6P 675198-71-7P 675198-73-9P
675198-74-0P, (1R,2S)-1-[[3,6-Diethy1-5-[(3-methylpyridin-2-y1)oxy]pyrazin-2-y1]amino]indan-2-o1 675198-75-1P
675198-77-3P 675198-78-4P 675198-80-8P
675198-81-9P, 1-[[3,6-Diethy1-5-[(4-methylphenyl)amino]pyrazin-2-y1]amino]indan-2-o1 675198-82-0P, N-(2-Ethoxy-2,3-dihydro-1H-inden-1-y1)-3,6-diethy1-5-[(4-methylphenyl)thio]pyrazin-2-amine
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of substituted 1,4-pyrazine derivs. as CRF inhibitors) 675198-67-1 CAPLUS

CN Pyrazinamine, N-[(1R,2S)-2-ethoxy-2,3-dihydro-1H-inden-1-yl]-3,6-diethyl-5-[(4-methyl-2-pyridinyl)oxy]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 675198-68-2 CAPLUS

CN Pyrazinamine, 3,6-diethyl-N-[(1R,2S)-2-(2-fluoroethoxy)-2,3-dihydro-1H-inden-1-yl]-5-[(4-methyl-2-pyridinyl)oxy]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 675198-69-3 CAPLUS

CN Pyrazinamine, N-[(1R,2S)-2,3-dihydro-2-(1-methylethoxy)-1H-inden-1-yl]-3,6-diethyl-5-[(4-methyl-2-pyridinyl)oxy]- (9CI) (CA INDEX NAME)

RN 675198-70-6 CAPLUS

CN Pyrazinamine, N-[(1R,2S)-2,3-dihydro-2-propoxy-1H-inden-1-y1]-3,6-diethyl-5-[(4-methyl-2-pyridinyl)oxy]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 675198-71-7 CAPLUS

CN 1H-Inden-2-ol, 1-[[3,6-diethyl-5-[(4-methyl-2-pyridinyl)oxy]pyrazinyl]amino]-2,3-dihydro-, acetate (ester), (1R,2S)-(9CI) (CA INDEX NAME)

RN 675198-73-9 CAPLUS

CN Pyrazinamine, N-[(1R,2S)-2-ethoxy-2,3-dihydro-1H-inden-1-yl]-3,6-diethyl-5-[(4-ethyl-2-pyridinyl)oxy]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 675198-74-0 CAPLUS

CN 1H-Inden-2-ol, 1-[[3,6-diethyl-5-[(3-methyl-2-pyridinyl)oxy]pyrazinyl]amino]-2,3-dihydro-, (1R,2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 675198-75-1 CAPLUS

CN Pyrazinamine, N-[(1R,2S)-2-ethoxy-2,3-dihydro-1H-inden-1-y1]-3,6-diethyl-5-[(3-methyl-2-pyridinyl)oxy]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 675198-77-3 CAPLUS

CN Pyrazinamine, N-[(1R,2S)-2-ethoxy-2,3-dihydro-1H-inden-1-yl]-3,6-diethyl-5-[(5-methyl-2-pyridinyl)oxy]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 675198-78-4 CAPLUS

CN Pyrazinamine, 5-[(4,6-dimethyl-2-pyridinyl)oxy]-N-[(1R,2S)-2-ethoxy-2,3-dihydro-1H-inden-1-yl]-3,6-diethyl- (9CI) (CA INDEX NAME)

RN 675198-80-8 CAPLUS

CN Pyrazinamine, N-[(1R,2S)-2-ethoxy-2,3-dihydro-1H-inden-1-yl]-3,6-diethyl-5-(3-methylphenoxy)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 675198-81-9 CAPLUS

CN 1H-Inden-2-ol, 1-[[3,6-diethyl-5-[(4-methylphenyl)amino]pyrazinyl]amino]-2,3-dihydro-(9CI) (CA INDEX NAME)

RN 675198-82-0 CAPLUS

CN Pyrazinamine, N-(2-ethoxy-2,3-dihydro-1H-inden-1-y1)-3,6-diethyl-5-[(4methylphenyl)thio]- (9CI) (CA INDEX NAME)

REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

ANSWER 3 OF 7 CAPLUS COPYRIGHT 2007 ACS on STN

1998:614437 CAPLUS ACCESSION NUMBER:

DOCUMENT NUMBER: 129:295965

TITLE: Organic electroluminescent device with high luminance

and polycyclic phosphorescent compound therefor

Onikubo, Shunichi; Tamano, Michiko; Okutsu, Satoshi; Enokida, Toshio INVENTOR(S):

PATENT ASSIGNEE(S): Toyo Ink Mfg. Co., Ltd., Japan SOURCE:

Jpn. Kokai Tokkyo Koho, 59 pp.

CODEN: JKXXAF

DOCUMENT TYPE: Patent LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

GI

PA:	TENT :	NO.			KINI)	DATE			APE	PLIC	ATI	: ИО	. O <i>l</i>			DA	TE	
JP	1025	1633			 A	_	1998	0922		JP	199	7-6	2568	3		•	19	970	317
JP	3503	403			В2		2004	0308											
EP	8661	10			A1		1998	0923		ΕP	199	8-3	0198	36			19	980	317
EP	8661	10			В1		2004	1020											
	R:	AT,	BE,	CH,	DE,	DK,	ES,	FR,	GB,	GF	۲, I	Τ,	LI,	LU,	NL,	SE	Ξ,	MC,	PT,
		ΙE,	SI,	LT,	LV,	FI,	, RO												
EP	9349	92			A1		1999	0811		ΕP	199	9-1	0669	98			19	980	317
EP	9349	92			В1		2004	0721											
	R:	DE,	FR,	GB															
US	6280	859			В1		2001	0828		US	199	8-4	2569	9			19	980	317
US	2001	0339	44		A1		2001	1025											
PRIORITY	APP	LN.	INFO	. :						JΡ	199	7-6	2568	3		Α	19	970	317
										EΡ	199	8-3	0198	36		А3	19	980	317
OTHER SO	OURCE	(S):			MARI	PAT	129:	29596	55										

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

The claimed compound is I [A = aromatic (condensed) ring, (condensed) AΒ heterocycle excluding Q1 (E = H or linkage), bivalent group comprising ≥ 2 kinds of 2-10 above ring systems which are connected directly or via O, N, S, C1-20 chain, nonarom. cycle, where the case of A = Q3 is excluded; Ar1-4 = (condensed) aromatic group; X1-4 = O, S, CO, SO2, CxH2xOCyH2y (x, y = 0-20; x + y \neq 0), C2-20 alkyl(id)ene, bivalent alicyclic group; R1-20 = H, halo, alkyl (oxy), aromatic ring, aromatic heterocycle, amino]. Also claimed is an organic electroluminescent device containing I with high luminance and good stability in repeated uses.

IT 213968-96-8

RL: DEV (Device component use); TEM (Technical or engineered material use); USES (Uses)

(luminescent material; organic electroluminescent device containing polycyclic

phosphorescent compound with high luminance)

RN 213968-96-8 CAPLUS

CN 2,5-Pyrazinedicarbonitrile, 3,6-bis[bis[4-(1-methyl-1phenylethyl)phenyl]amino]- (CA INDEX NAME)

L4 ANSWER 4 OF 7 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1992:571474 CAPLUS

DOCUMENT NUMBER: 117:171474

TITLE: Cyanopyrazine derivatives and their manufacture

INVENTOR(S): Kojima, Takakazu

PATENT ASSIGNEE(S): Nippon Soda Co., Ltd., Japan SOURCE: Jpn. Kokai Tokkyo Koho, 4 pp.

CODEN: JKXXAF

DOCUMENT TYPE: Patent LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 04112877	A	19920414	JP 1990-232592	19900904
PRIORITY APPLN. INFO.:			JP 1990-232592	19900904
OTHER SOURCE(S):	CASREA	ACT 117:17147	74; MARPAT 117:171474	
GI				

AB Title derivs. I [R = alkyl, aralkyl, cycloalkyl, alkenyl, (substituted) aryl] are manufactured by dimerizing II in the presence of an oxidation catalyst.

Thus, dimerization of II (R = Ph) in 1,2-dimethoxyethane/H2O in the

presence of E.C. 1.11.1.7 and H2O2 under ice cooling for 5 h gave 54% I (R = Ph).

IT 143469-44-7P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of, by dimerization of diamino(chlorophenylthio)acrylonitrile)

RN 143469-44-7 CAPLUS

CN Pyrazinecarbonitrile, 5,6-diamino-3-[(4-chlorophenyl)thio]- (9CI) (CA INDEX NAME)

IT 143469-43-6P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of, by dimerization of diamino(phenylthio)acrylonitrile)

RN 143469-43-6 CAPLUS

CN Pyrazinecarbonitrile, 5,6-diamino-3-(phenylthio)- (9CI) (CA INDEX NAME)

IT 143469-45-8P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of, by dimerization of diamino(tolylthio)acrylonitrile)

RN 143469-45-8 CAPLUS

CN Pyrazinecarbonitrile, 5,6-diamino-3-[(4-methylphenyl)thio]- (9CI) (CA INDEX NAME)

L4 ANSWER 5 OF 7 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1984:139145 CAPLUS

DOCUMENT NUMBER: 100:139145

ORIGINAL REFERENCE NO.: 100:21243a, 21246a

TITLE: 2-Amino derivatives of 3-chloro-5-nitro-6-

aminopyrazines useful as adjuncts to radiation therapy

INVENTOR(S): Hartman, George D.

PATENT ASSIGNEE(S): Merck and Co., Inc. , USA

SOURCE: U.S., 4 pp. Cont.-in-part of U.S. Ser. No. 295,446,

abandoned.
CODEN: USXXAM

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
				-	
US 4418062	A	19831129	US 1982-399924		19820719
PRIORITY APPLN. INFO.:			US 1980-194100	A2	19801006
			US 1981-295446	A2	19810824
OTHER SOURCE(S):	CASREA	CT 100:13914	45; MARPAT 100:139145)	

C102N.

GΙ

AΒ 2,6-Pyrazinediamines I (R and R1 are alkyl, hydroxyalkyl, aminoalkyl, substituted alkenyl, or NRR1 from a saturated heterocycle), useful as tumor cell sensitizers (no data), were prepared 5,6-Dichloro-3-nitro-2pyrazinamine was treated with H2NCH2CH2OH and Et3N to give I (R = H, R1 = CH2CH2OH).

ΙT 88793-48-0P

> RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of)

RN 88793-48-0 CAPLUS

CN 2,6-Pyrazinediamine, 3-chloro-5-nitro-N2-phenyl- (CA INDEX NAME)

ANSWER 6 OF 7 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1981:208189 CAPLUS

DOCUMENT NUMBER: 94:208189

94:34043a,34046a ORIGINAL REFERENCE NO.:

TITLE: Theoretical estimation of pKa values of

pyrazinylquanidine derivatives

AUTHOR(S): Bock, Mark G.; Schlegel, H. Bernard; Smith, Graham M. CORPORATE SOURCE: Merck, Sharp and Dohme Res. Lab., West Point, PA,

19486, USA

SOURCE: Journal of Organic Chemistry (1981), 46(9), 1925-7

CODEN: JOCEAH; ISSN: 0022-3263

DOCUMENT TYPE: Journal English LANGUAGE:

AΒ The pKa values of substituted anilines and pyridines were predicted equally well by semiempirical and minimal basis set ab initio methods. CNDO/2 calcns. on the diuretic amiloride and closely related derivs. gave a practical correlation between calculated proton affinities and measured solution-phase pKa values.

70296-90-1 ΙT

RL: PRP (Properties)

(basicity constant and proton affinity of, MO calcn. of)

RN 70296-90-1 CAPLUS

CN Pyrazinecarboxamide, 3,5-diamino-N-(aminoiminomethyl)-6-(phenylthio)-(9CI) (CA INDEX NAME)

$$\begin{array}{c|c} \text{O} & \text{NH} \\ || & || \\ \text{C-NH-C-NH}_2 \\ \\ \text{H}_2 \text{N} & \text{NH}_2 \end{array}$$

L4 ANSWER 7 OF 7 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1979:204142 CAPLUS

DOCUMENT NUMBER: 90:204142

ORIGINAL REFERENCE NO.: 90:32485a,32488a

TITLE: Amiloride and its 6-substituted derivatives

PATENT ASSIGNEE(S): Merck and Co., Inc., USA SOURCE: Jpn. Kokai Tokkyo Koho, 6 pp.

CODEN: JKXXAF

DOCUMENT TYPE: Patent LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 54012389	A	19790130	JP 1978-79240	19780629
US 4196292	A	19800401	US 1977-811011	19770629
FI 7801966	A	19781230	FI 1978-1966	19780620
HU 20578	A2	19810828	HU 1978-ME2174	19780622
ни 178302	В	19820428		
PL 119097	B1	19811130	PL 1978-207947	19780627
DK 7802902	A	19781230	DK 1978-2902	19780628
NO 7802230	A	19790102	NO 1978-2230	19780628
EP 200	A1	19790110	EP 1978-100264	19780628
EP 200	B1	19820324		
R: BE, CH, DE,	FR, GB	, LU, NL, SE		
ES 471244	A1	19791001	ES 1978-471244	19780628
AT 7804690	A	19801115	AT 1978-4690	19780628
AT 362795	В	19810610		
PRIORITY APPLN. INFO.:			US 1977-811011	A 19770629
OTHER SOURCE(S):	MARPAT	90:204142		
GI				

Amilorides I (R = R1; R1 = C1, CN, SMe, SCF3,SPh) were prepared by treating I (R = Br, iodo) with CuR1 in OP(NMe2)3 (or DMF) or by amidation of II (R1 as above; R2 = OMe) with guanidine. I (R = R1) are diuretics, antihypertensives and antiinflammatory agents (5-750 mg/day). Thus, treatment of 3.5 g I.HCl (R = iodo) with CuCN in OP(NMe2)3 15 min at 100° gave 1.43 g I (R = CN).

IT 70296-94-5

RL: RCT (Reactant); RACT (Reactant or reagent) (amidation of, with guanidine)

RN 70296-94-5 CAPLUS

CN Pyrazinecarboxylic acid, 3,5-diamino-6-(phenylthio)-, methyl ester (9CI)

70296-90-1P ΙT

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation and diuretic, hypotensive and antiinflammatory activities of)

RN 70296-90-1 CAPLUS

CN Pyrazinecarboxamide, 3,5-diamino-N-(aminoiminomethyl)-6-(phenylthio)-(9CI) (CA INDEX NAME)

=> log hold COST IN U.S. DOLLARS

SINCE FILE TOTAL SESSION

FULL ESTIMATED COST

ENTRY 212.49 40.18

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE TOTAL

CA SUBSCRIBER PRICE

ENTRY SESSION -5.46-5.46

SESSION WILL BE HELD FOR 120 MINUTES STN INTERNATIONAL SESSION SUSPENDED AT 07:21:42 ON 28 DEC 2007

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Welcome to STN International! Enter x:x

LOGINID:ssspta1623zct

* * * * * RECONNECTED TO STN INTERNATIONAL * * * * * * SESSION RESUMED IN FILE 'CAPLUS' AT 07:54:48 ON 28 DEC 2007 FILE 'CAPLUS' ENTERED AT 07:54:48 ON 28 DEC 2007 COPYRIGHT (C) 2007 AMERICAN CHEMICAL SOCIETY (ACS)

COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	40.18	212.49

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) SINCE FILE TOTAL

ENTRY SESSION CA SUBSCRIBER PRICE -5.46 -5.46

=> file reg

COST IN U.S. DOLLARS SINCE FILE TOTAL ENTRY SESSION

FULL ESTIMATED COST 40.18 212.49

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) SINCE FILE TOTAL ENTRY SESSION

CA SUBSCRIBER PRICE -5.46 -5.46

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TSCA INFORMATION NOW CURRENT THROUGH June 29, 2007

Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

http://www.cas.org/support/stngen/stndoc/properties.html

=> =>

=>

=> file reg
COST IN U.S. DOLLARS
SINCE FILE TOTAL
ENTRY SESSION

FULL ESTIMATED COST 0.90 213.39

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE
ENTRY
SESSION

CA SUBSCRIBER PRICE 0.00 -5.46

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STRUCTURE FILE UPDATES: 27 DEC 2007 HIGHEST RN 959655-61-9 DICTIONARY FILE UPDATES: 27 DEC 2007 HIGHEST RN 959655-61-9

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH June 29, 2007

Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

http://www.cas.org/support/stngen/stndoc/properties.html

=>

Uploading C:\Program Files\Stnexp\Queries\10649299.str



chain nodes:
7 9 10 11 13
ring nodes:
1 2 3 4 5 6
chain bonds:
2-11 3-13 5-10 6-7 7-9
ring bonds:
1-2 1-6 2-3 3-4 4-5 5-6
exact/norm bonds:
2-11 3-13 5-10 6-7 7-9
normalized bonds:
1-2 1-6 2-3 3-4 4-5 5-6

G1:0,S,N

G2:C,O,S

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 9:Atom 10:CLASS 11:CLASS 13:CLASS

Generic attributes :

9:

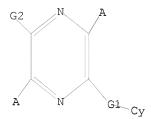
Saturation : Unsaturated

L5 STRUCTURE UPLOADED

=> d 15

L5 HAS NO ANSWERS

L5 STR



G1 O, S, N

G2 C, O, S

Structure attributes must be viewed using STN Express query preparation.

=> s 15

SAMPLE SEARCH INITIATED 07:56:19 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 3505 TO ITERATE

57.1% PROCESSED 2000 ITERATIONS

RATIONS

6 ANSWERS

INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 66550 TO 73650

PROJECTED TIERATIONS: 66550 TO 73650 PROJECTED ANSWERS: 16 TO 404

L6 6 SEA SSS SAM L5

=> d 1-6

L6 ANSWER 1 OF 6 REGISTRY COPYRIGHT 2007 ACS on STN

RN 139964-69-5 REGISTRY

ED Entered STN: 27 Mar 1992

CN Benzoic acid, 3-[(3-chloro-5,6-dicyanopyrazinyl)amino]- (9CI) (CA INDEX NAME)

MF C13 H6 C1 N5 O2

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L6 ANSWER 2 OF 6 REGISTRY COPYRIGHT 2007 ACS on STN

RN 128142-29-0 REGISTRY

ED Entered STN: 13 Jul 1990

CN Pyrazinecarbonitrile, 5,6-dimethyl-3-(phenylsulfinyl)- (9CI) (CA INDEX NAME)

MF C13 H11 N3 O S

SR CA

LC STN Files: CA, CAPLUS

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L6 ANSWER 3 OF 6 REGISTRY COPYRIGHT 2007 ACS on STN

RN 72545-94-9 REGISTRY

ED Entered STN: 16 Nov 1984

CN 2,3-Pyrazinedicarbonitrile, 5-methyl-6-(3-methylphenoxy)- (CA INDEX NAME)

MF C14 H10 N4 O

LC STN Files: CA, CAPLUS

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L6 ANSWER 4 OF 6 REGISTRY COPYRIGHT 2007 ACS on STN

RN 72545-78-9 REGISTRY

ED Entered STN: 16 Nov 1984

CN 2,3-Pyrazinedicarbonitrile, 5-chloro-6-[(3-chlorophenyl)amino]- (CA INDEX NAME)

MF C12 H5 C12 N5

LC STN Files: CA, CAPLUS, TOXCENTER

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1907 TO DATE)

2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L6 ANSWER 5 OF 6 REGISTRY COPYRIGHT 2007 ACS on STN

RN 72114-04-6 REGISTRY

ED Entered STN: 16 Nov 1984

CN 2,3-Pyrazinedicarbonitrile, 5-(ethylamino)-6-(3-methylphenoxy)- (CA INDEX NAME)

MF C15 H13 N5 O

LC STN Files: BEILSTEIN*, CA, CAPLUS

(*File contains numerically searchable property data)

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1907 TO DATE)

2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L6 ANSWER 6 OF 6 REGISTRY COPYRIGHT 2007 ACS on STN

RN 39870-63-8 REGISTRY

ED Entered STN: 16 Nov 1984

CN 2,6-Pyrazinedicarbonitrile, 3-amino-5-(methylphenylamino)- (CA INDEX NAME)

OTHER NAMES:

CN 2-Amino-3,5-dicyano-6-(N-methylanilino)pyrazine

MF C13 H10 N6

LC STN Files: BEILSTEIN*, CA, CAPLUS, IFICDB, IFIPAT, IFIUDB, USPATFULL, USPATOLD

(*File contains numerically searchable property data)

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1907 TO DATE)
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

=>

=> s 11 sss full FULL SEARCH INITIATED 07:58:20 FILE 'REGISTRY' FULL SCREEN SEARCH COMPLETED - 25778 TO ITERATE

100.0% PROCESSED 25778 ITERATIONS

50 ANSWERS

SEARCH TIME: 00.00.01

L7 50 SEA SSS FUL L1

=> file caplus

 COST IN U.S. DOLLARS
 SINCE FILE
 TOTAL

 ENTRY
 SESSION

 FULL ESTIMATED COST
 185.15
 398.54

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE TOTAL
ENTRY SESSION
CA SUBSCRIBER PRICE

0.00 -5.46

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=> s 17 L8

7 L7

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FILE 'REGISTRY' ENTERED AT 07:17:02 ON 28 DEC 2007

L1STRUCTURE UPLOADED

L2 2 S L1

L3 50 S L1 SSS FULL

FILE 'CAPLUS' ENTERED AT 07:17:35 ON 28 DEC 2007

L47 S L3

FILE 'REGISTRY' ENTERED AT 07:55:00 ON 28 DEC 2007

FILE 'REGISTRY' ENTERED AT 07:55:56 ON 28 DEC 2007

L5STRUCTURE UPLOADED

6 S L5 L6

L7 50 S L1 SSS FULL

FILE 'CAPLUS' ENTERED AT 07:58:28 ON 28 DEC 2007

L8 7 S L7

=> s 18 not 14

L9 0 L8 NOT L4

=> logoff

ALL L# QUERIES AND ANSWER SETS ARE DELETED AT LOGOFF

LOGOFF? (Y)/N/HOLD:y

SINCE FILE TOTAL ENTRY SESSION COST IN U.S. DOLLARS

FULL ESTIMATED COST 0.47 399.01

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) SINCE FILE TOTAL

> ENTRY SESSION

CA SUBSCRIBER PRICE -5.46 0.00

STN INTERNATIONAL LOGOFF AT 07:59:07 ON 28 DEC 2007